Supplementary Materials: Synthesis of Catechol Derived Rosamine Dyes and Their Reactivity toward Biogenic Amines

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NMR spectrum of 2,3-dibenzyloxybenzaldehyde and 3,4-dibenzyloxybenzaldehyde

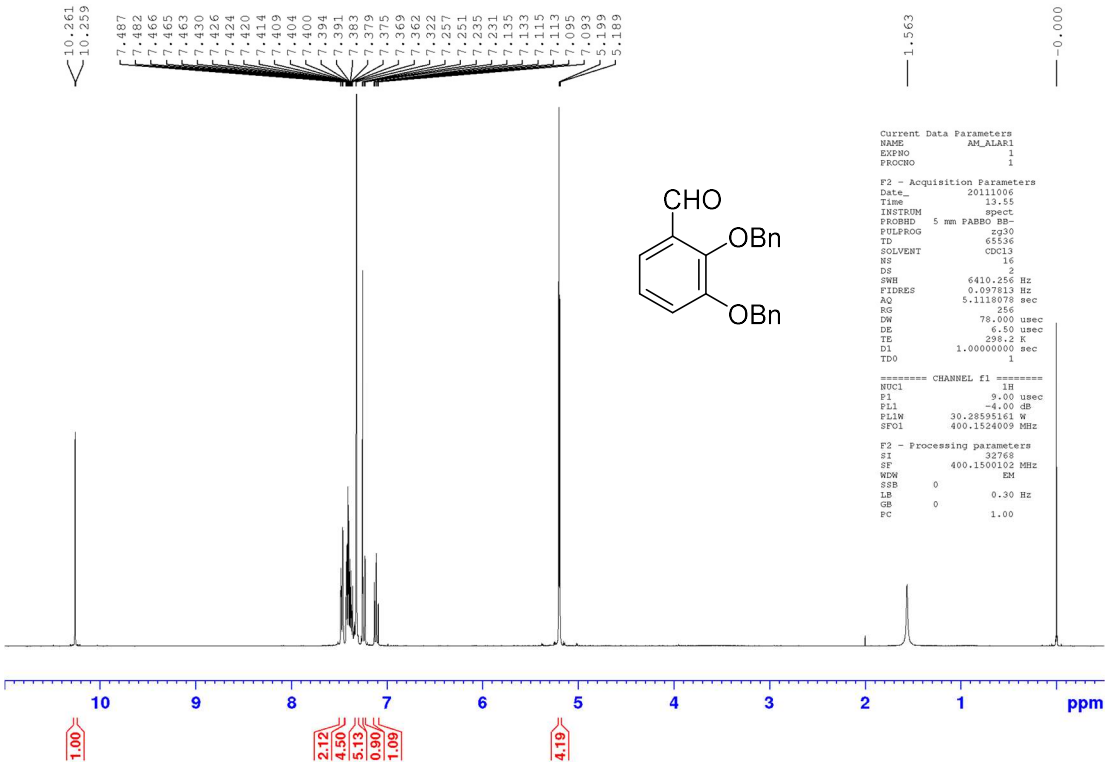


Figure S1. ^{1}H NMR spectrum (400.15 MHz, $CDCl_3$) of 2,3-dibenzyloxybenzaldehyde.

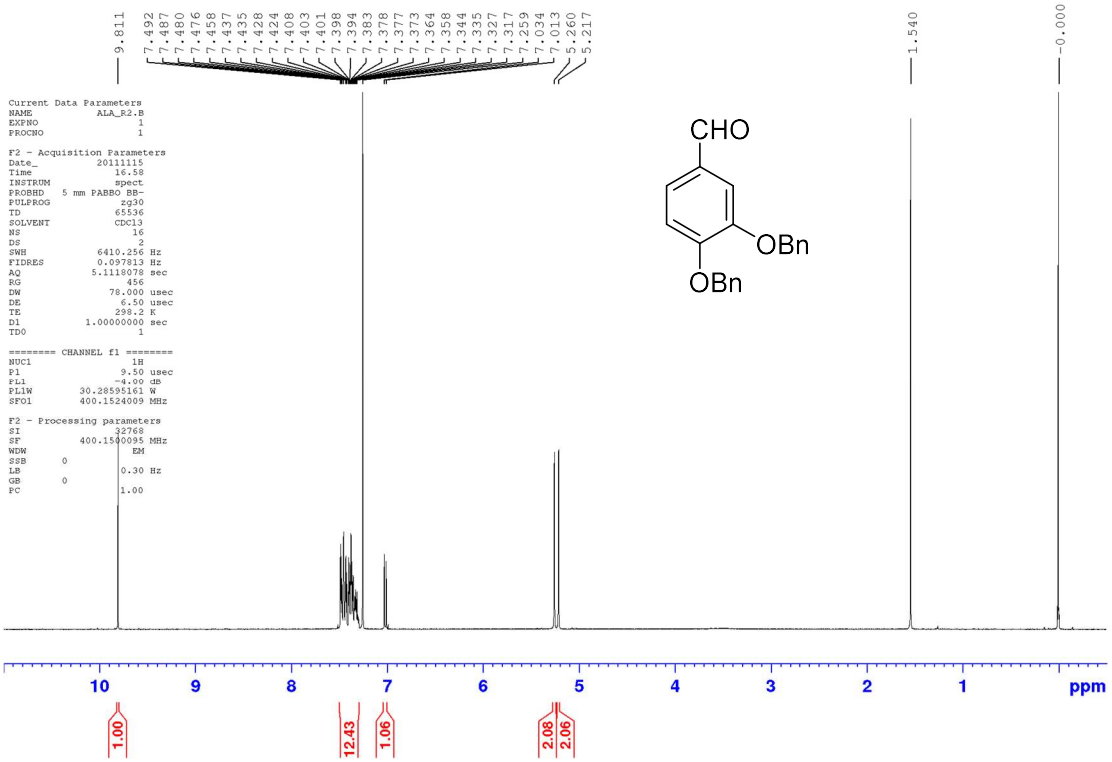


Figure S2. ^{1}H NMR spectrum (400.15 MHz, $CDCl_3$) of 3,4-dibenzyloxybenzaldehyde.

NMR spectra of rosamine 1

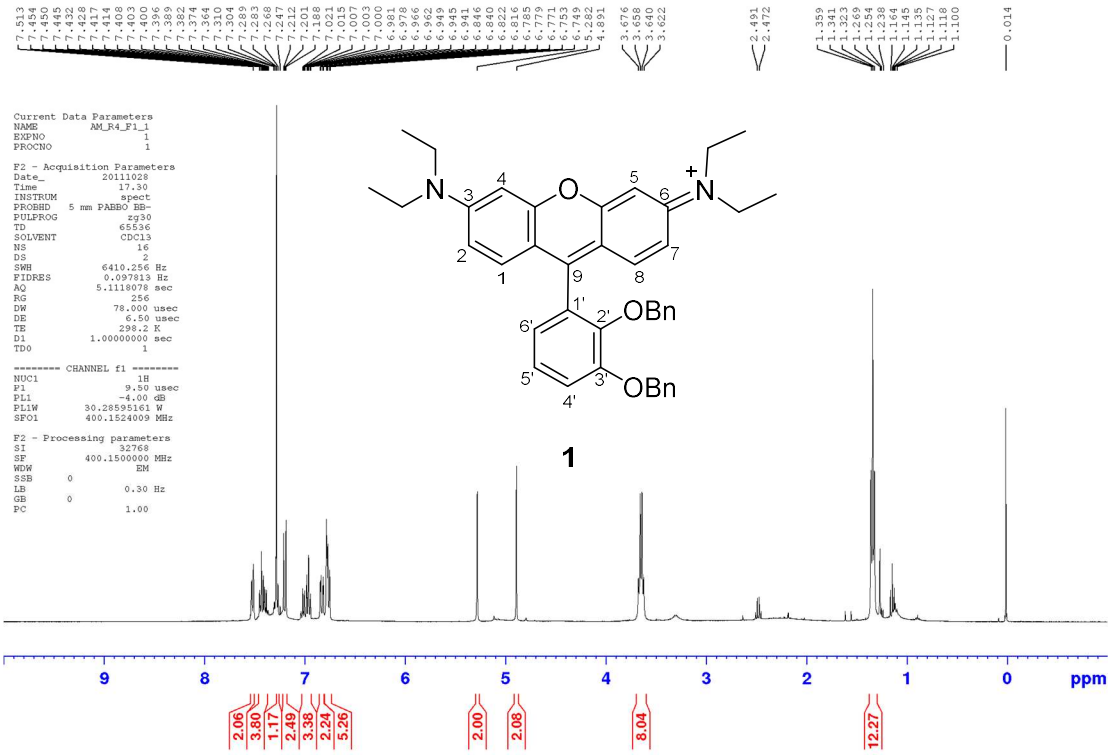


Figure S3. ^{1}H NMR spectrum (400.15 MHz, $CDCl_3$) of **1**.

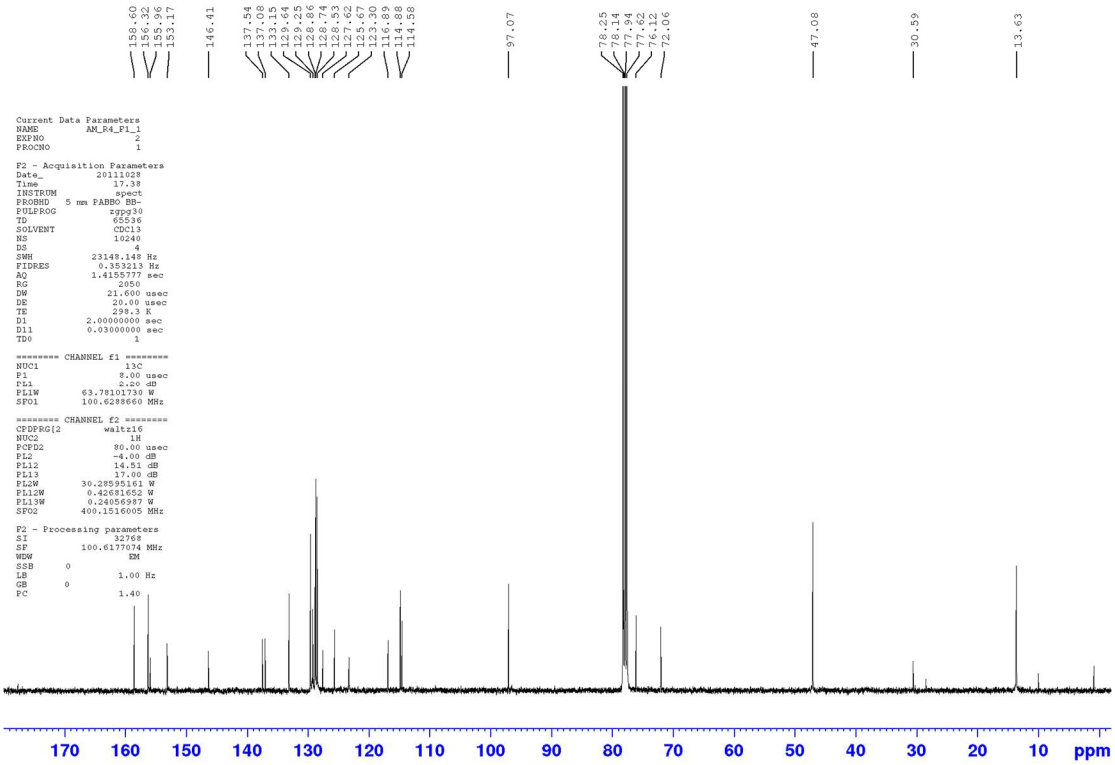


Figure S4. ^{13}C NMR spectrum (100.63 MHz, $CDCl_3$) of **1**.

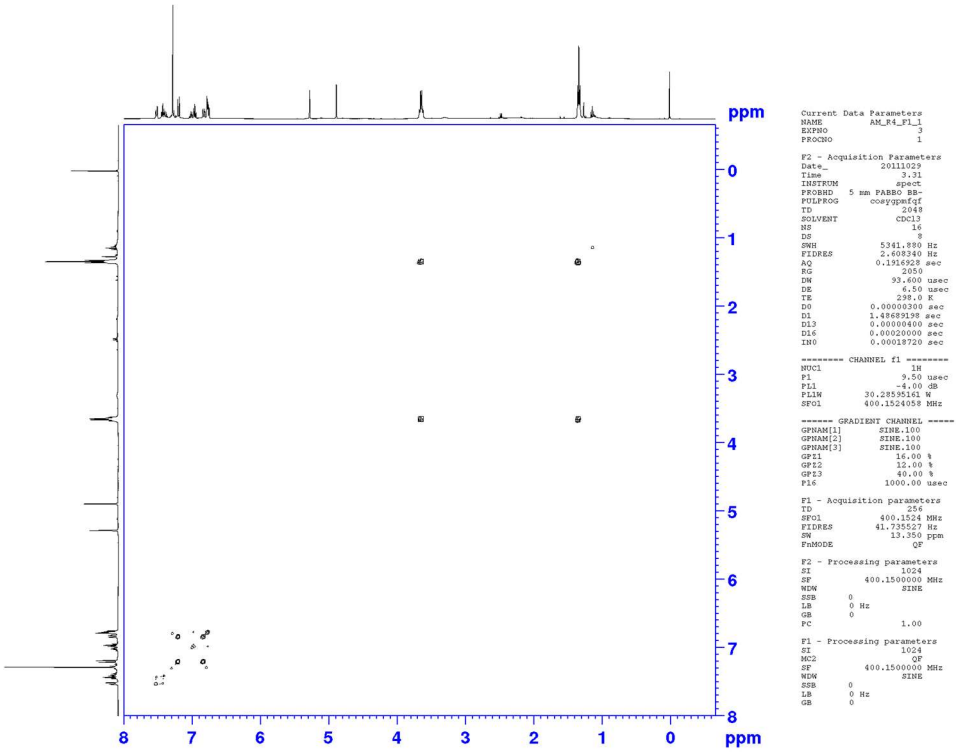


Figure S5. COSY spectrum of **1**.

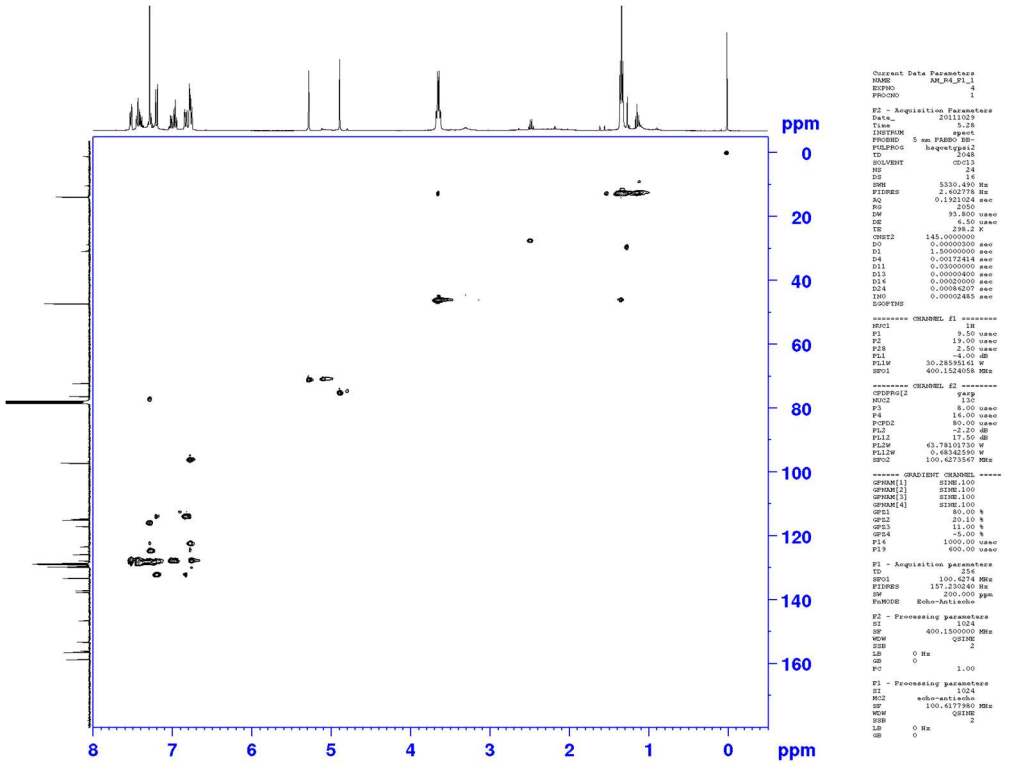


Figure S6. HSQC spectrum of **1**.

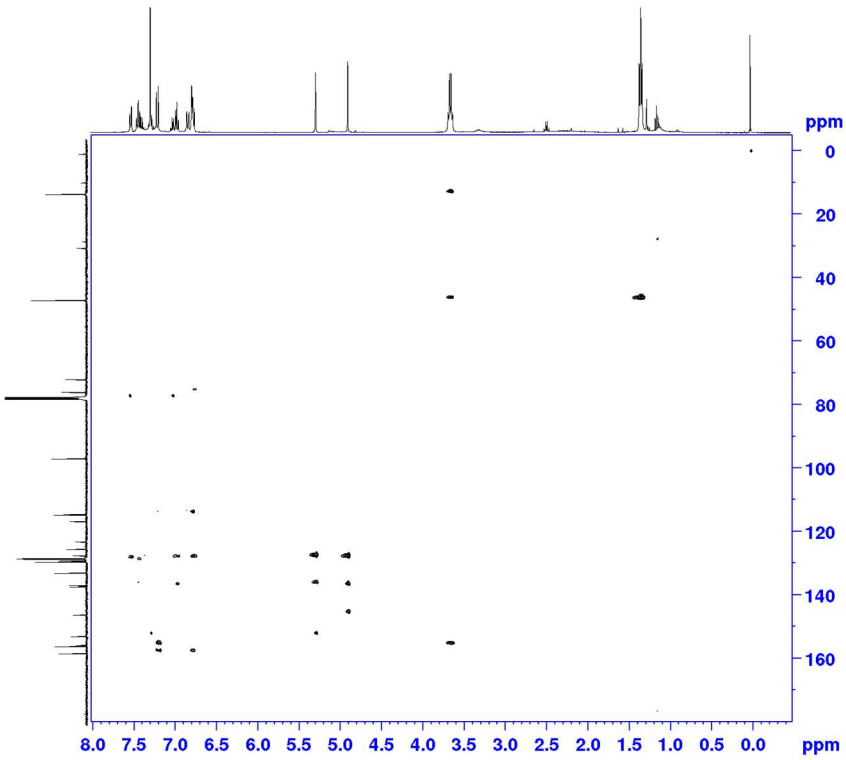


Figure S7. HMBC spectrum of **1**.

NMR spectra of rosamine 2

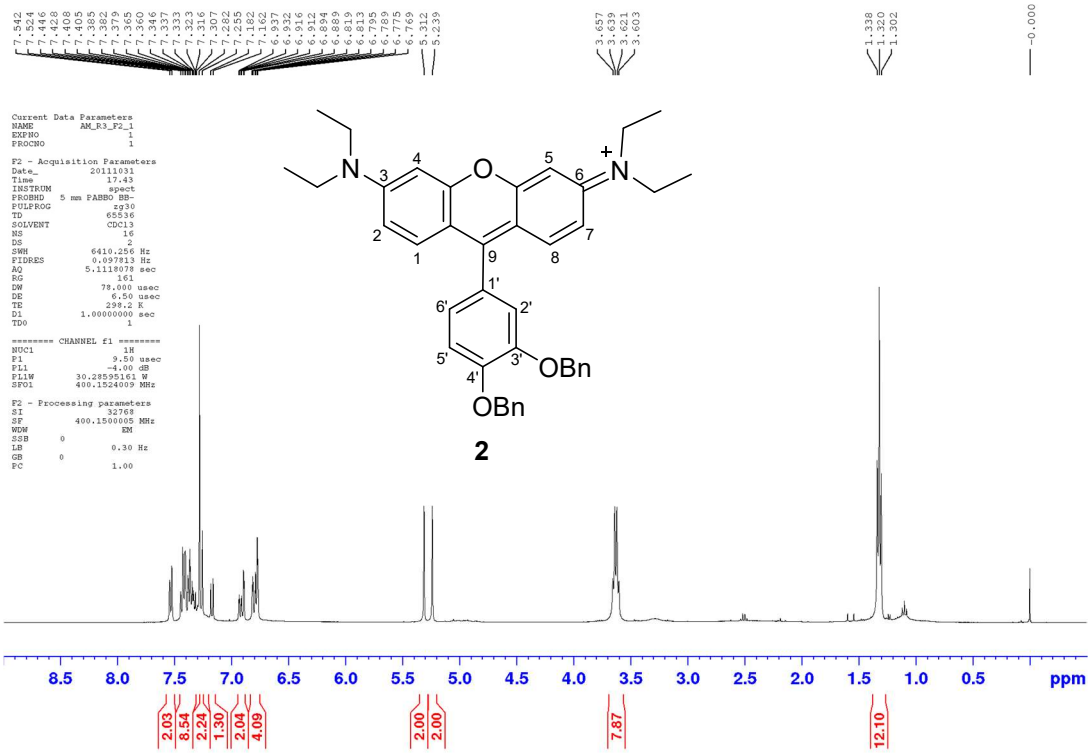


Figure S8. ^{1}H NMR spectrum (400.15 MHz, $CDCl_3$) of **2**.

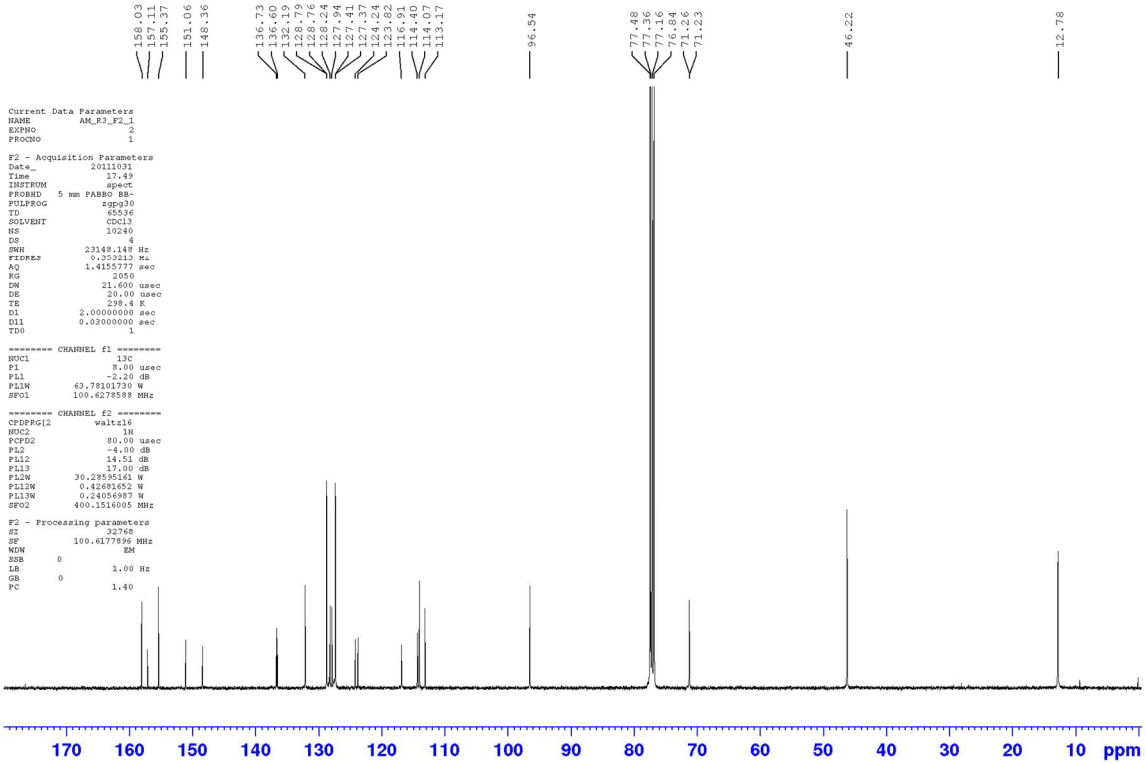


Figure S9. ^{13}C NMR spectrum (100.63 MHz, $CDCl_3$) of **2**.

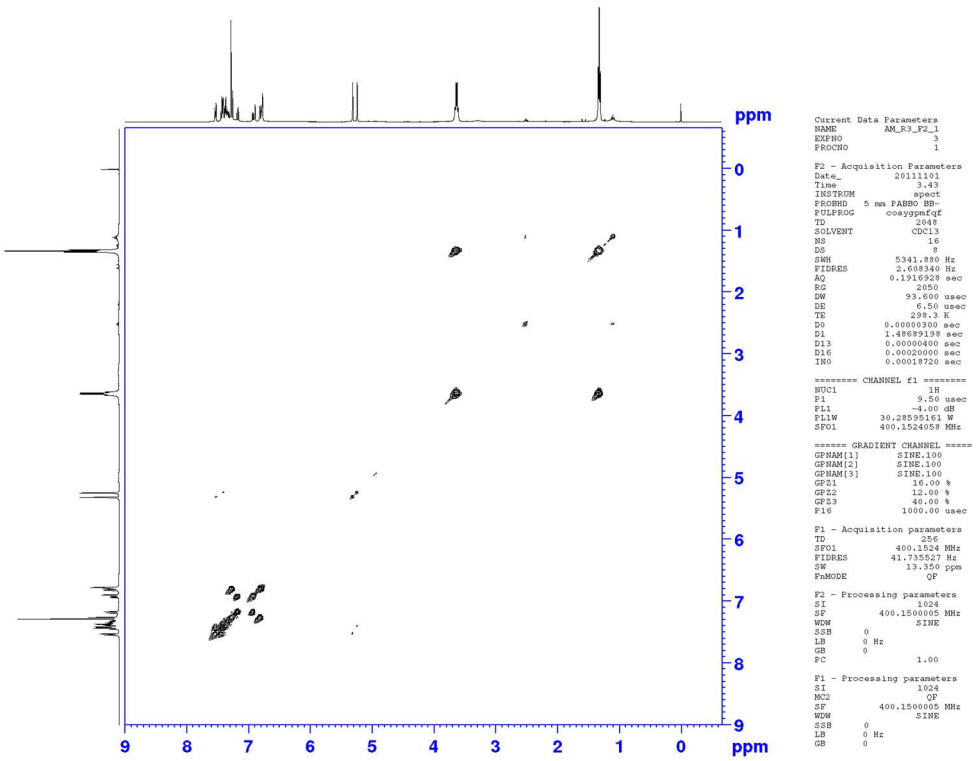


Figure S10. COSY spectrum of **2**.

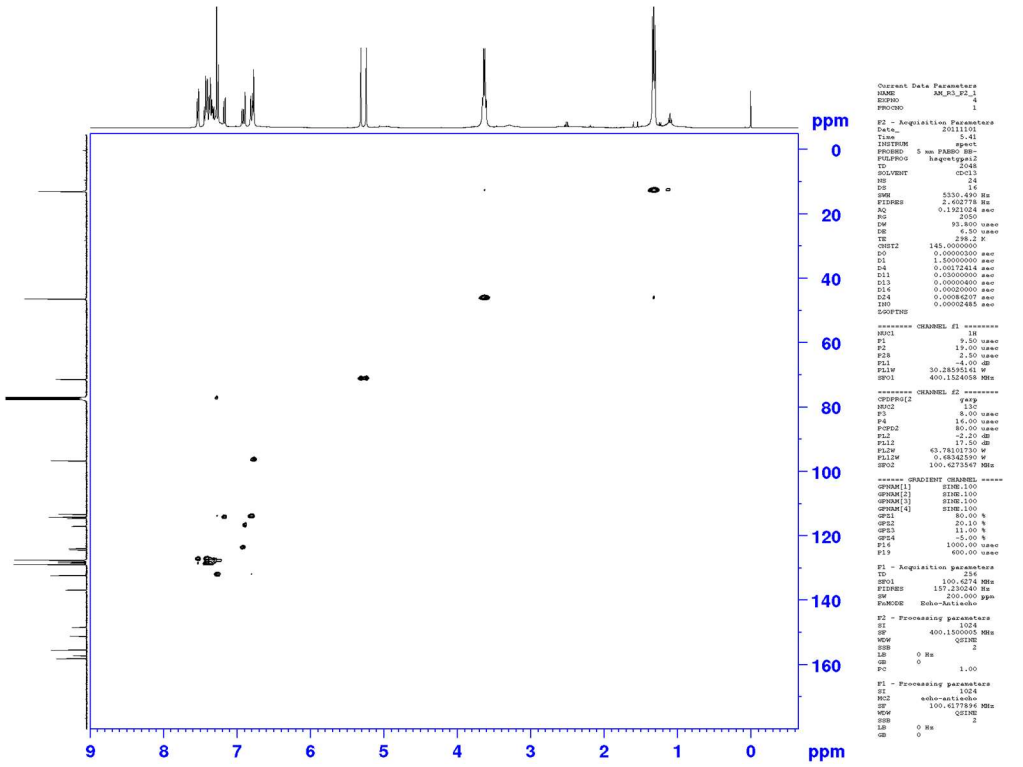


Figure S11. HSQC spectrum of **2**.

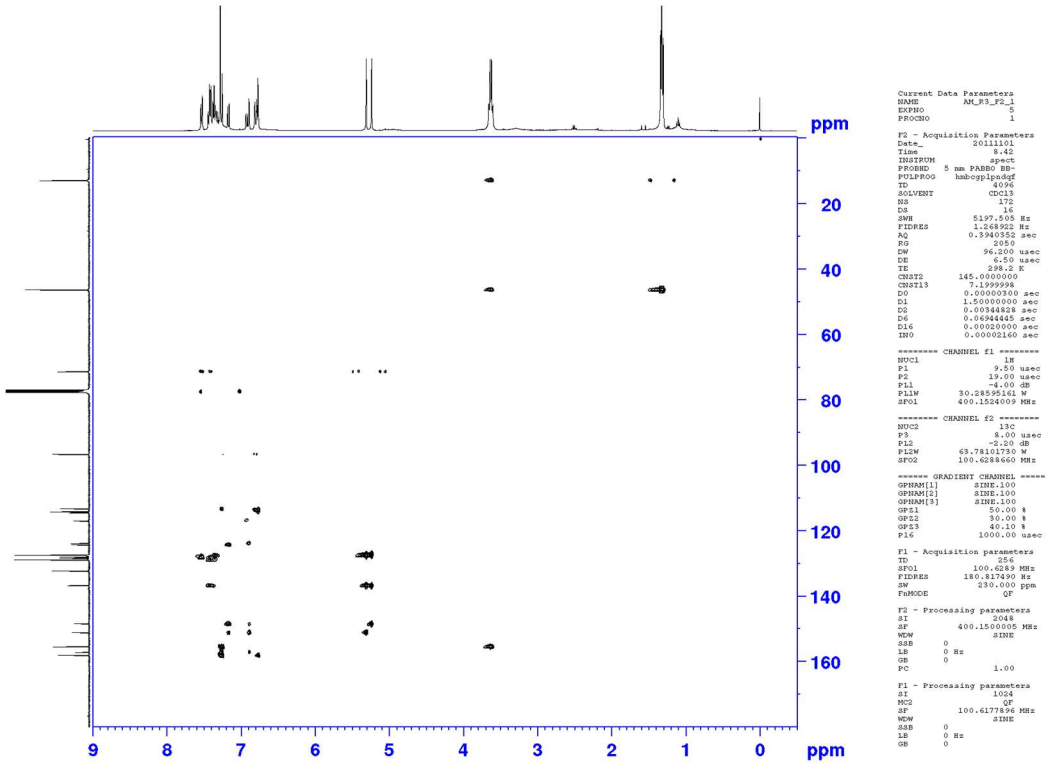


Figure S12. HMBC spectrum of **2**.

NMR spectra of rosamine 3

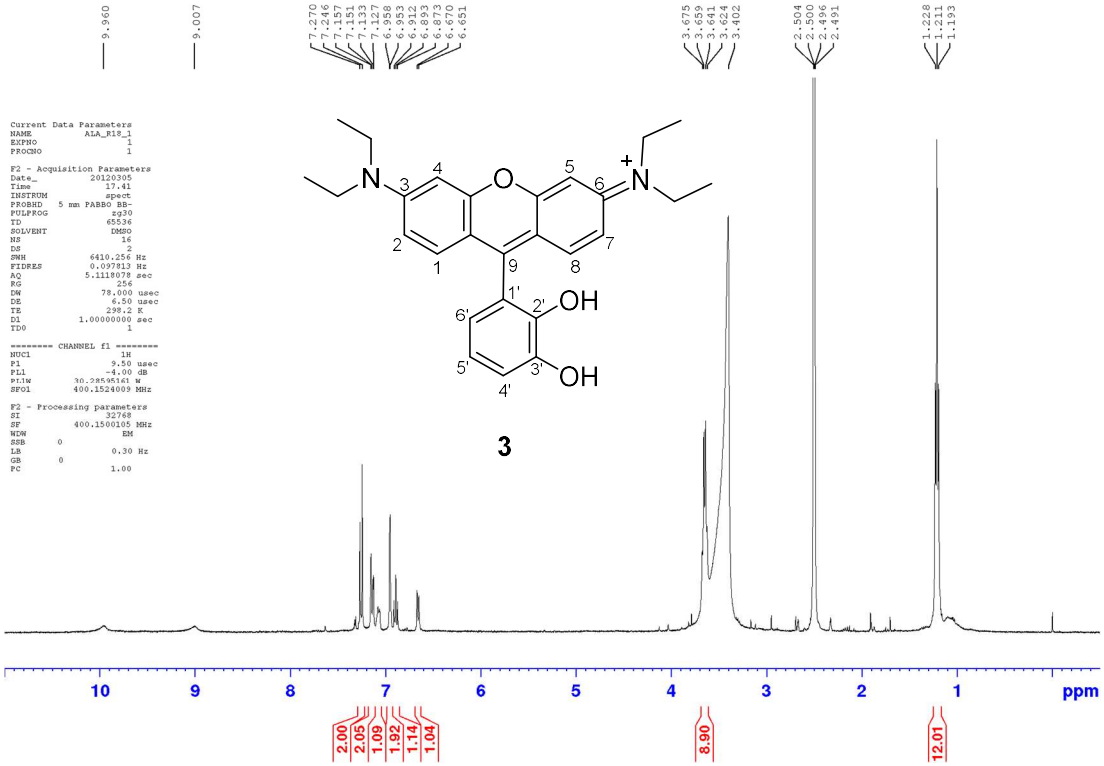


Figure S13. ^{1}H NMR spectrum (400.15 MHz, DMSO-d$_6$) of **3**.

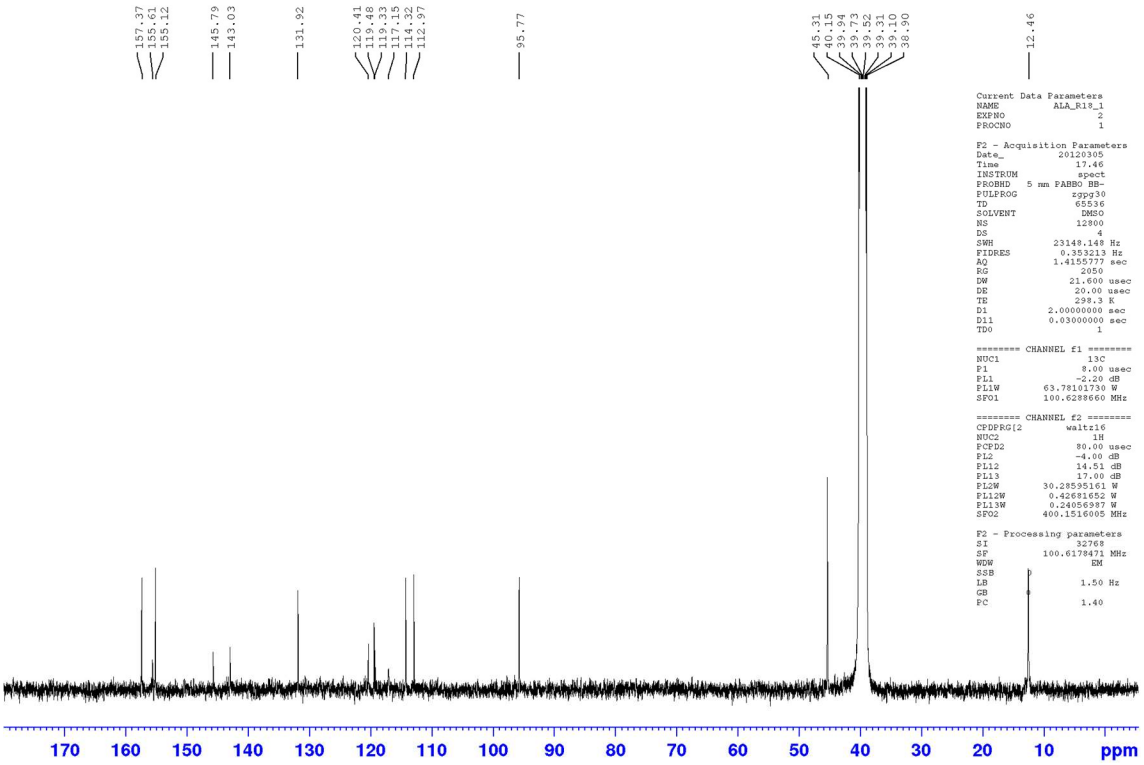


Figure S14. ^{13}C NMR spectrum (100.63 MHz, DMSO-d_6) of **3**.

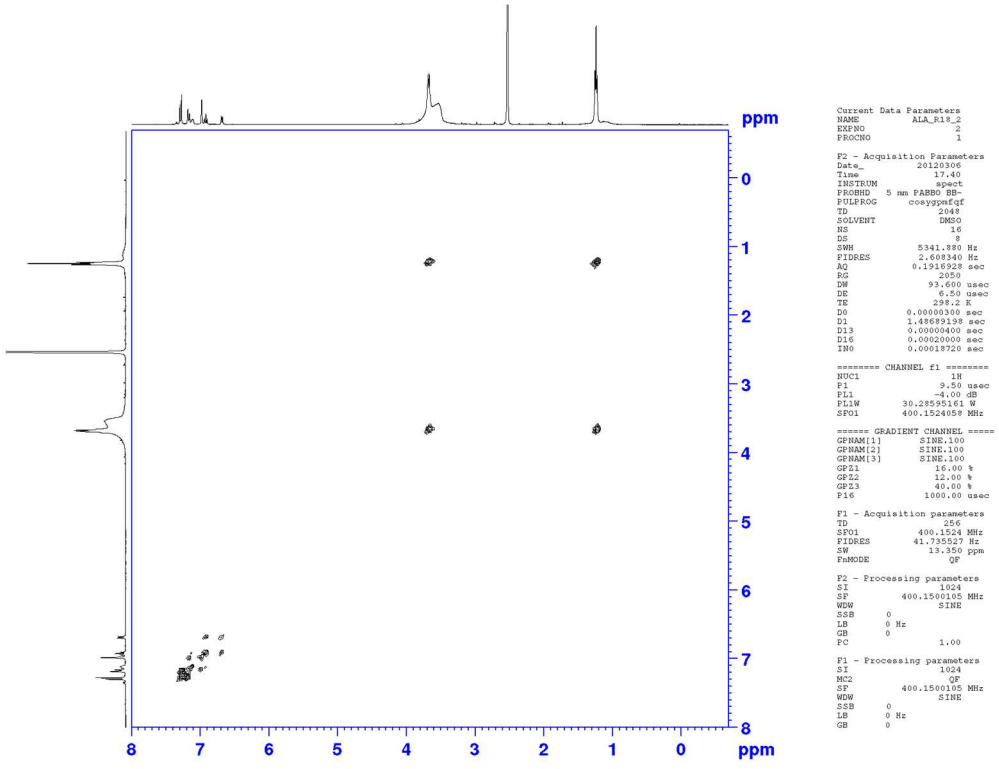


Figure S15. COSY spectrum of **3**.

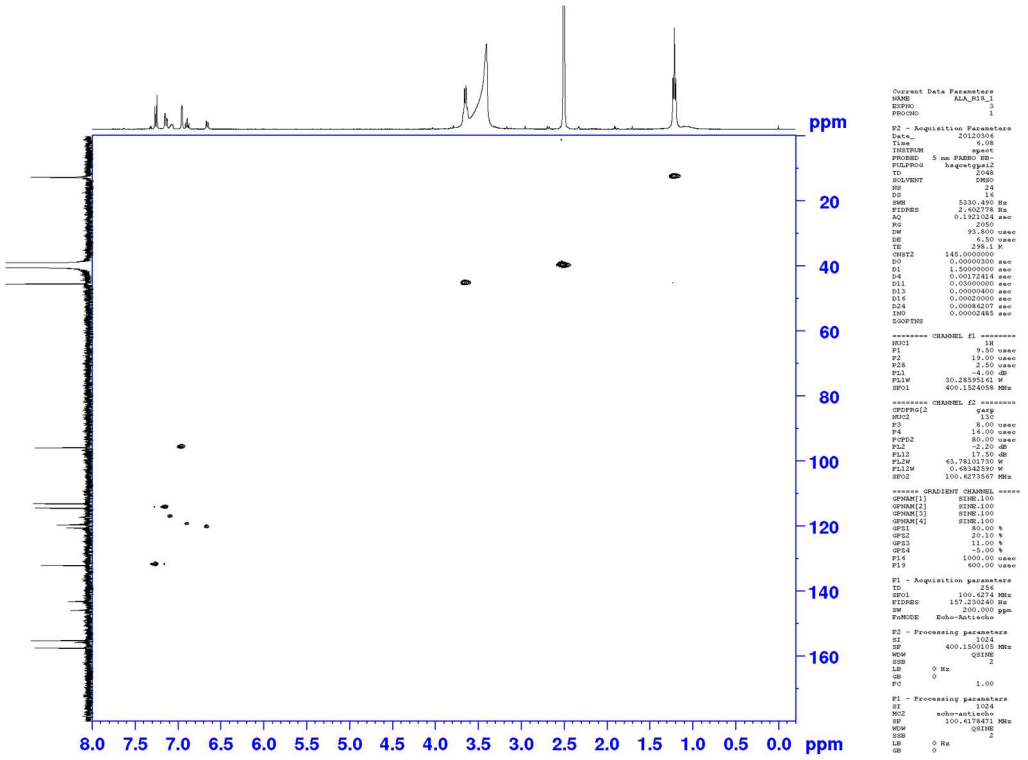


Figure S16. HSQC spectrum of **3**.

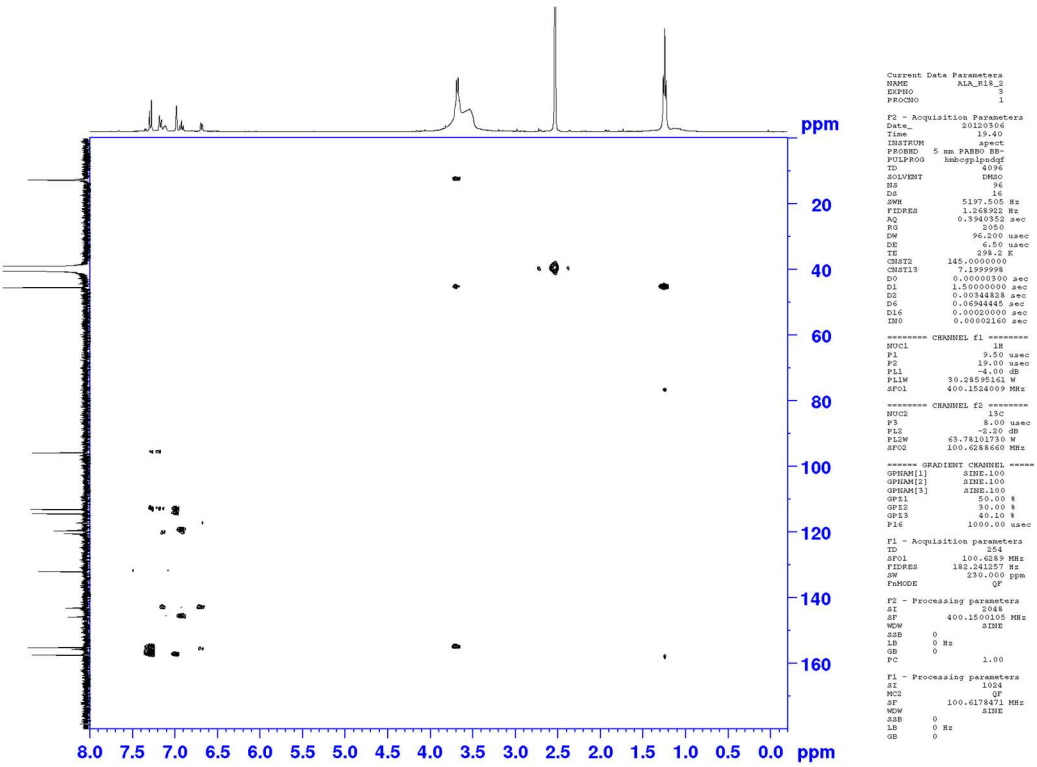


Figure S17. HMBC spectrum of **3**.

NMR spectra of rosamine 4

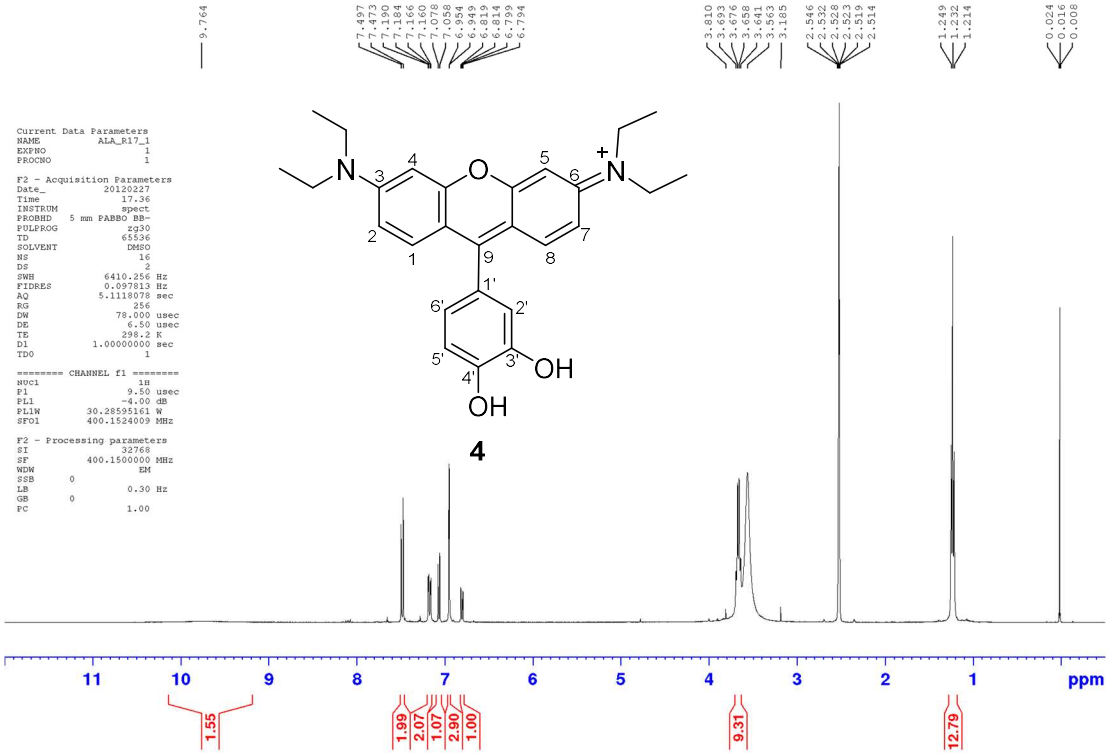


Figure S18. ^{1}H NMR spectrum (400.15 MHz, DMSO-d$_6$) of **4**.

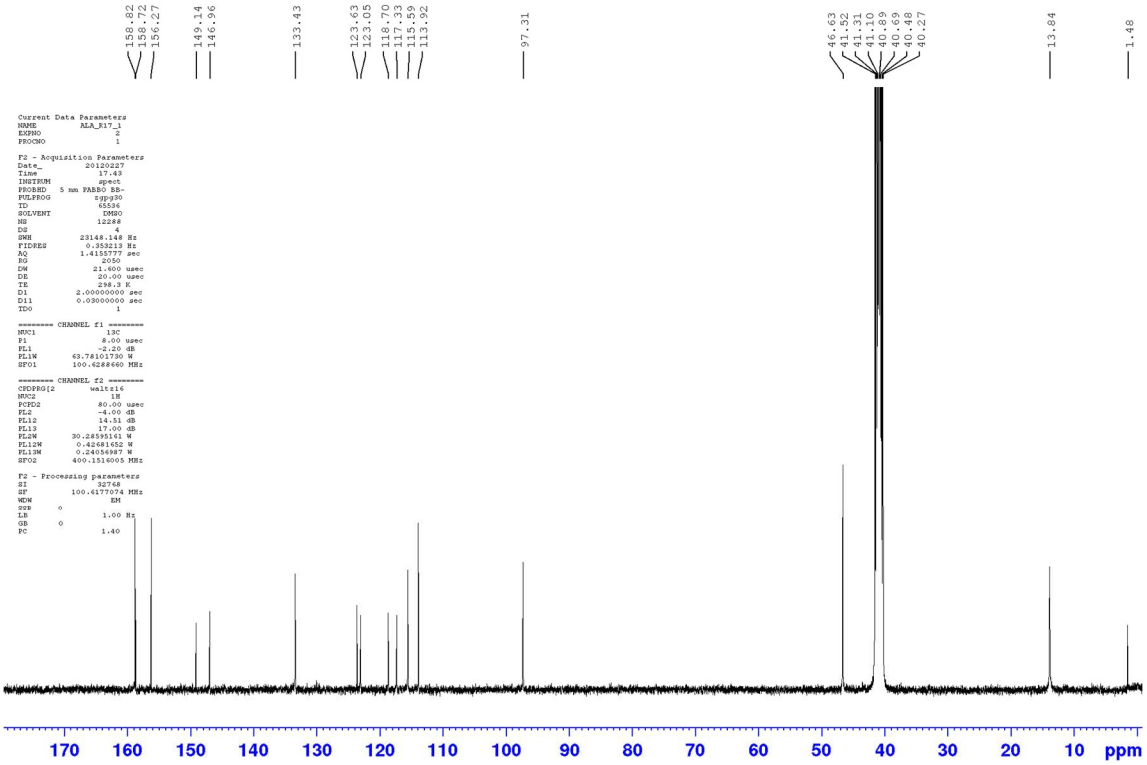


Figure S19. ^{13}C NMR spectrum (100.63 MHz, DMSO-d$_6$) of **4**.

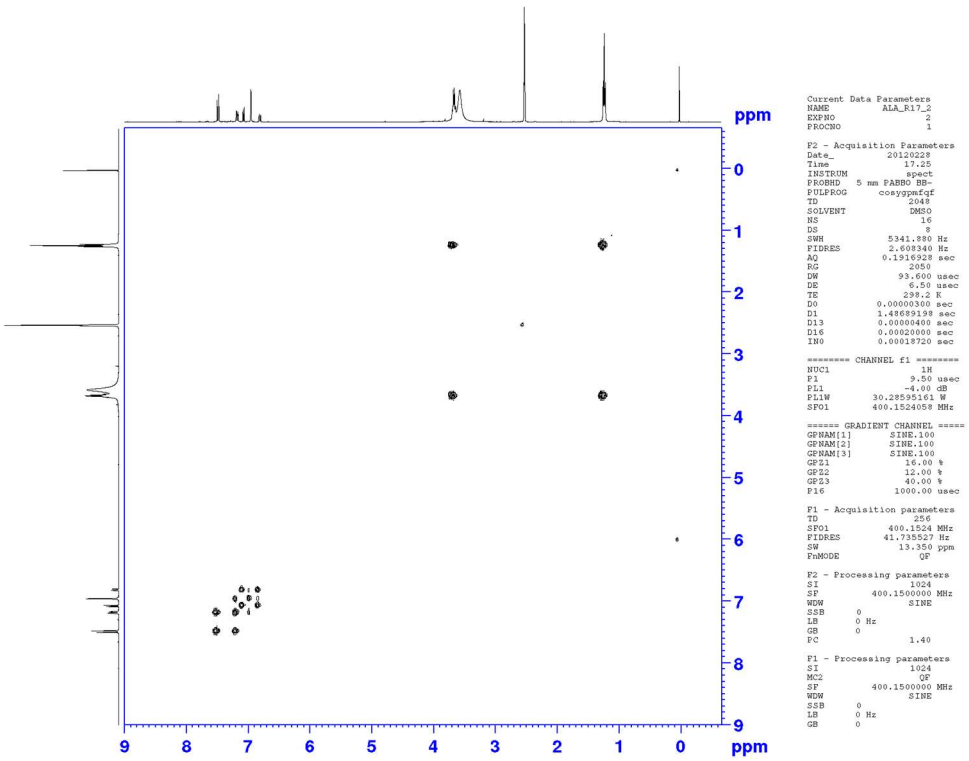


Figure S20. COSY spectrum of **4**.

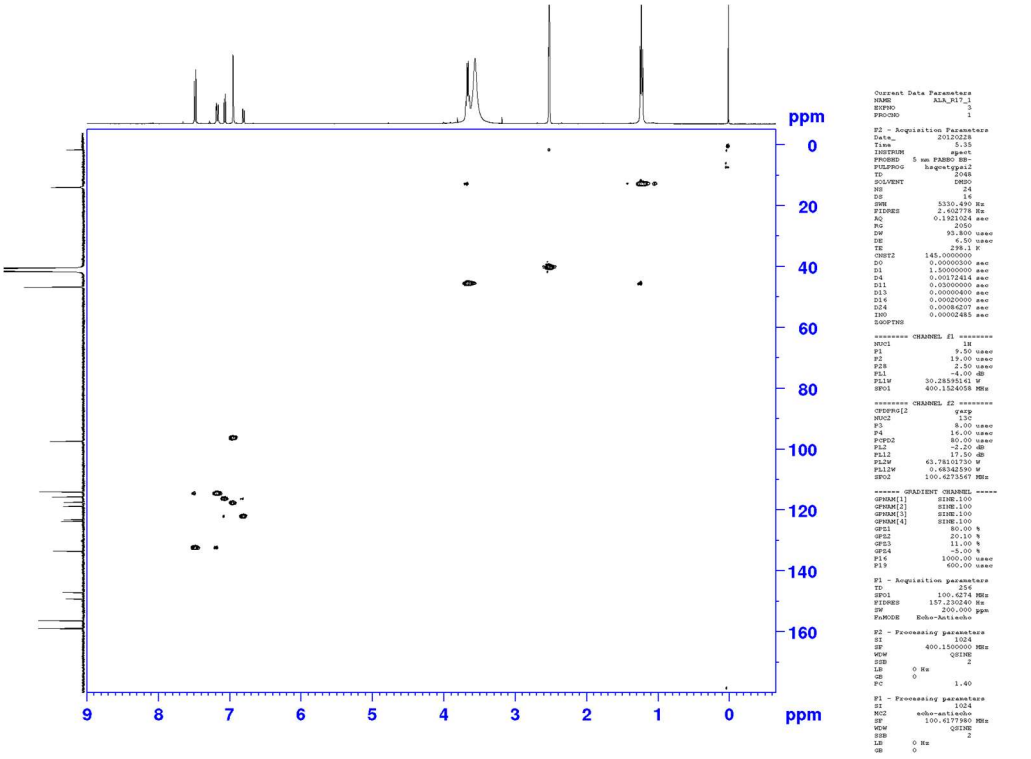


Figure S21. HSQC spectrum of **4**.

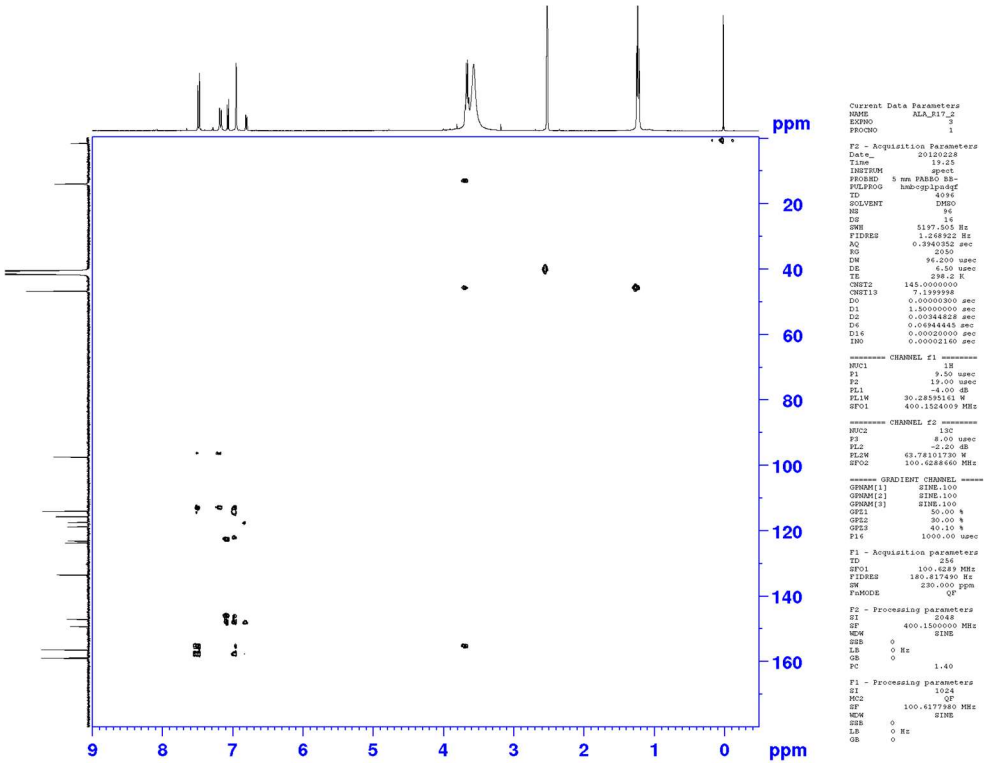


Figure S22. HMBC spectrum of **4**.

MS spectra of 1, 2, 3 and 4

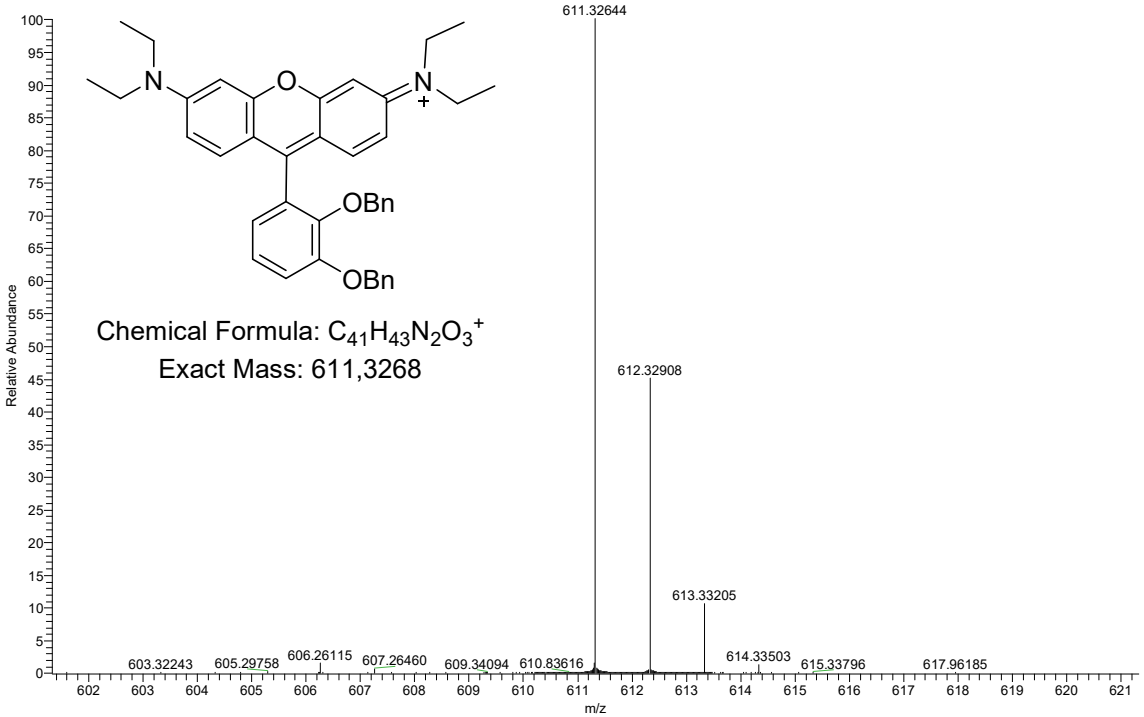


Figure S23. MS spectrum of **1**

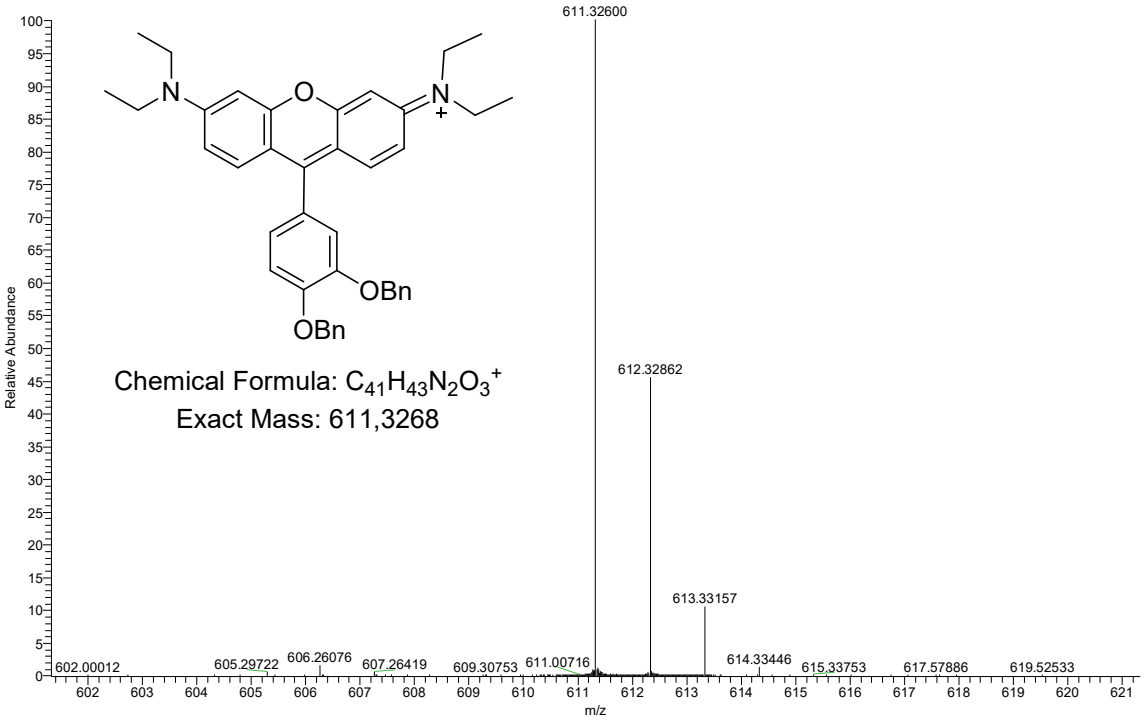


Figure S24. MS spectrum of **2**

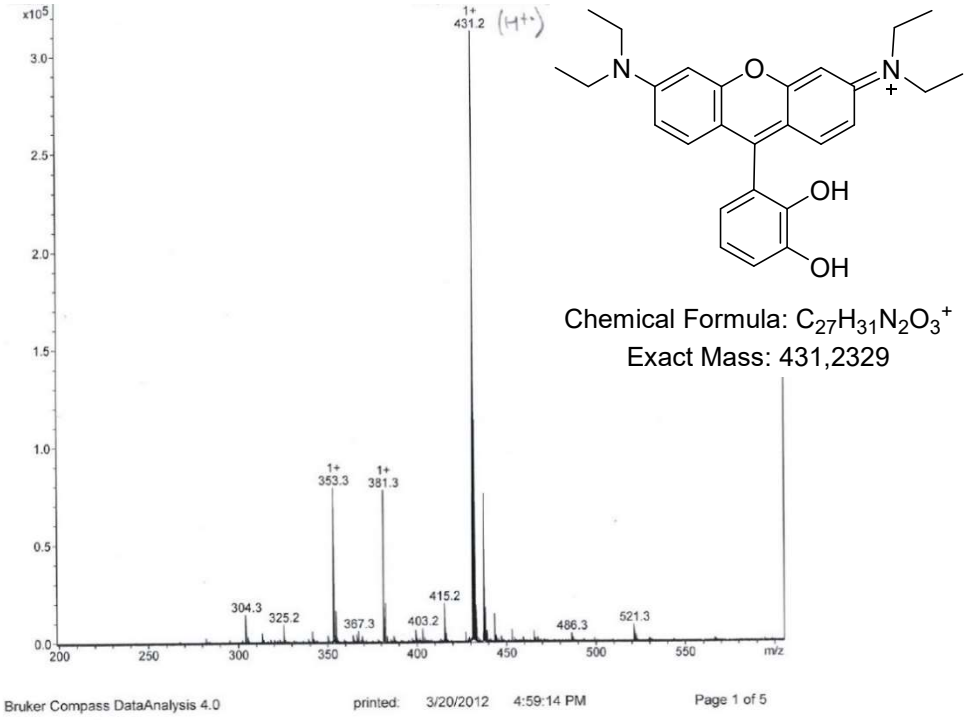
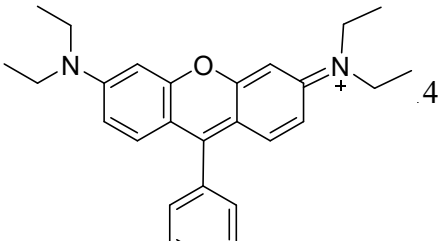


Figure S25. MS spectrum of **3**



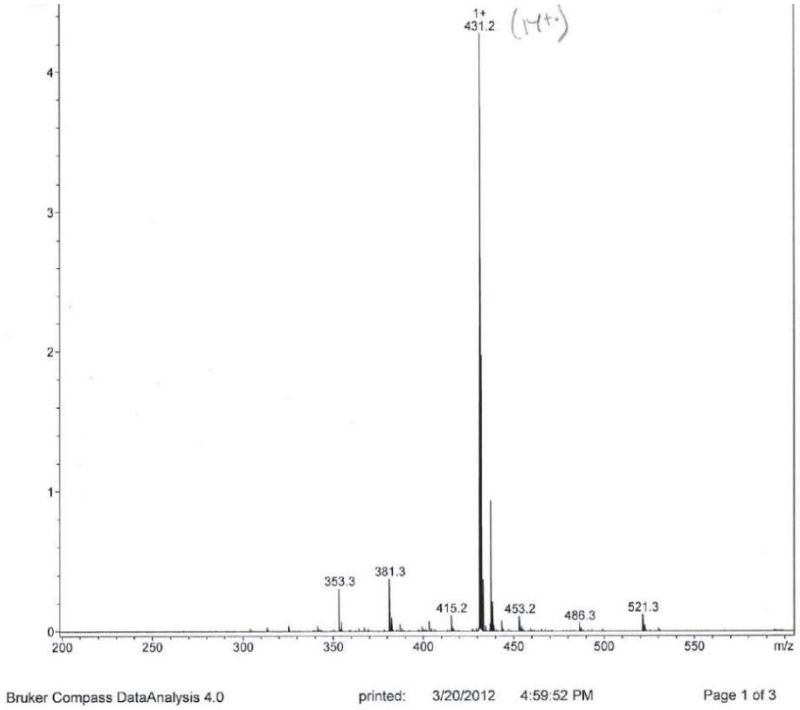


Figure S26. MS spectrum of **4**

The influence of pH variation in the fluorescence intensity of rosamine 4.

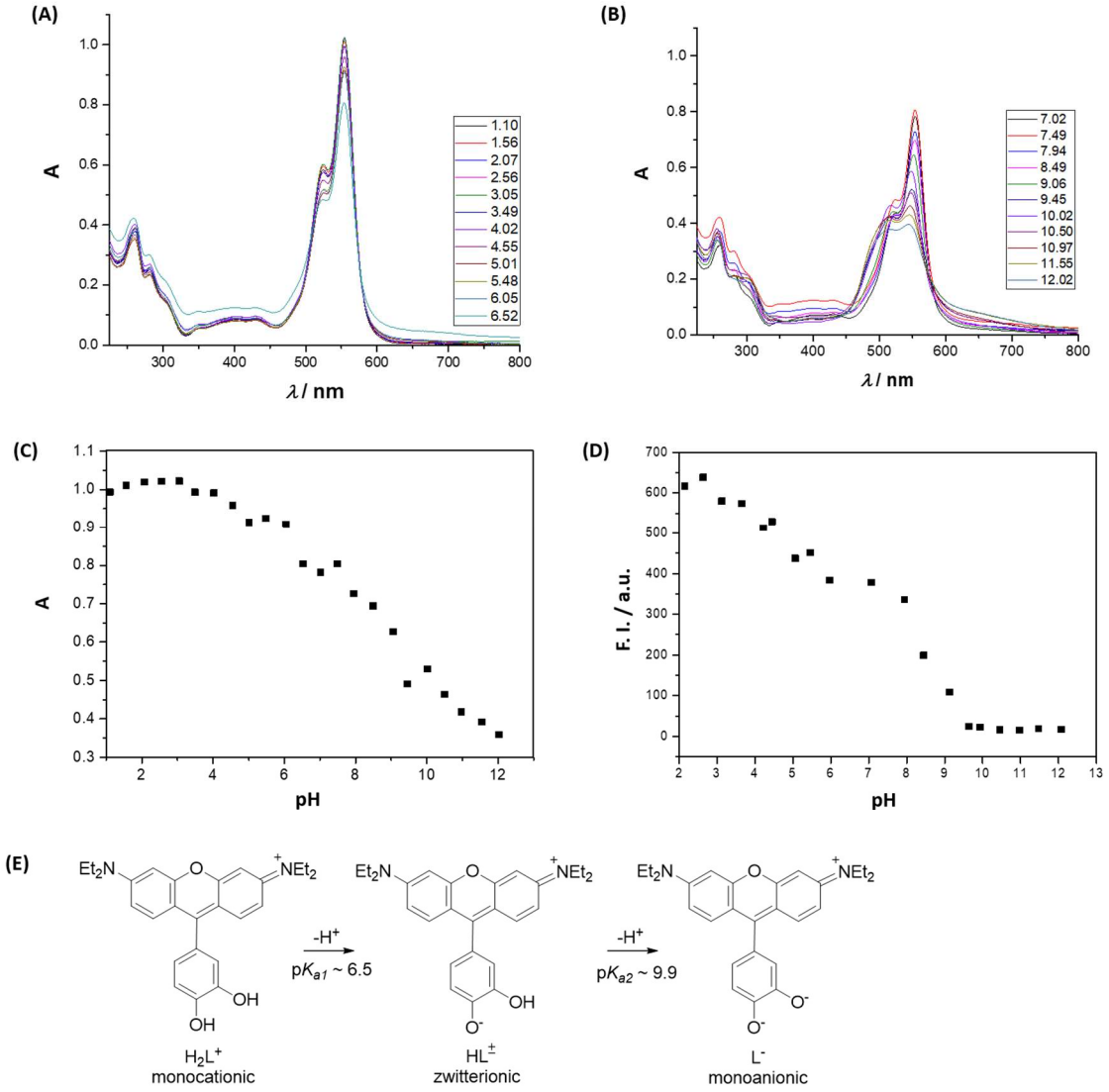


Figure S27. The influence of pH variation in the fluorescence intensity of rosamine **4**. A – Absorption spectra for pH < 7; B – Absorption spectra for pH ≥ 7); C – Graphical representation of the pH in function of the maximum in absorbance; D – Graphical representation of the pH as a function of the maximum in fluorescence intensity; E – Structures and pK_a's of rosamine **4** deprotonation.

Detection study of rosamine 4 with different biogenic amines in solution (preliminary study)

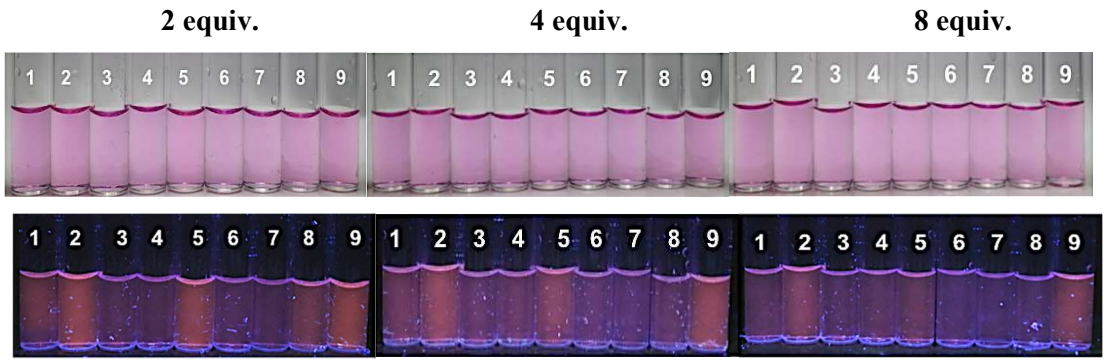


Figure S28. Samples with 2, 4 and 8 equiv. of 1-histamine, 2-tyramine, 3-cadaverine, 4-putrescine, 5-phenylethylamine, 6-spermidine, 7-spermine, 8-butylamine, 9- rosamine **4**, observed under visible (top) and UV light (bottom).

Detection study of rosamine 4 with different amines in solution (CH_3CN)

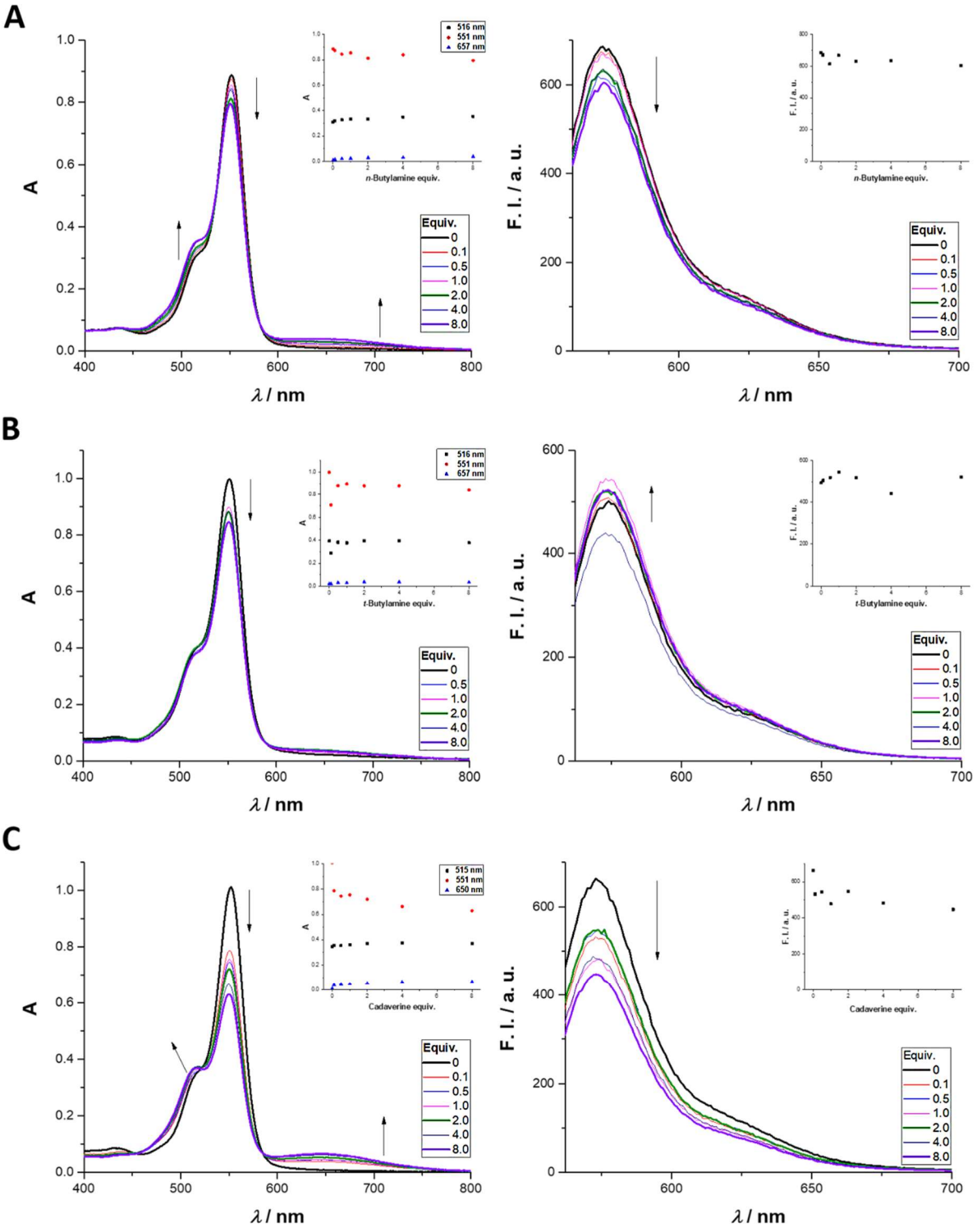


Figure S29. Absorption (left) and emission (right) spectra of **4** upon addition (0 – 8 equiv.) of *n*-butylamine (**A**), *t*-butylamine (**B**) and cadaverine (**C**) in CH_3CN (the inset graphs represent the variation in absorbance (right) and fluorescence intensity (left) for the wavelengths that present more variation in intensity. |**4**| = 35 μM and λ_{exc} = 551 nm.

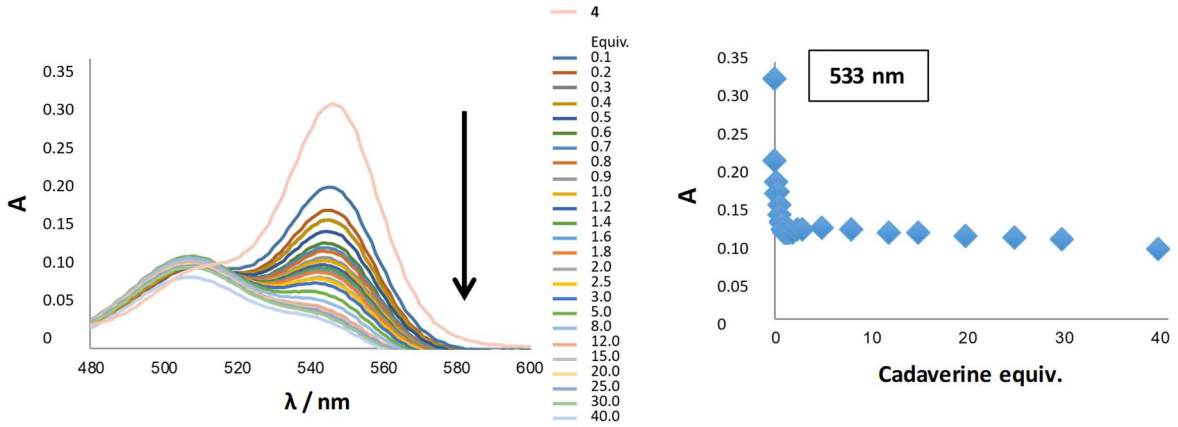


Figure S30. Absorption (left) spectrum of **4** upon addition (0.1–40 equiv.) of cadaverine in CH_3CN and graph representing the variation in absorbance (right) intensity at 533 nm |4| = 5 μM.

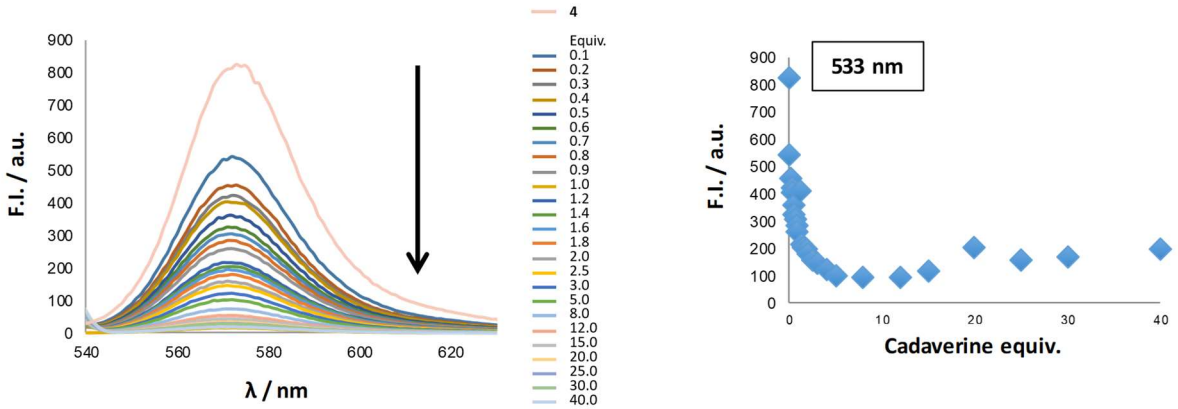


Figure S31. Emission (left) spectrum of **4** upon addition (0.1–40 equiv.) of cadaverine in CH_3CN and graph representing the variation in emission (right) intensity |4| = 5 μM and λ_{exc} = 533 nm.

Detection study of rosamine 4 with different biogenic amines in gas phase

Figure S32. Commercial biogenic amine samples subjected to heat

NMR spectra of aminopyronin 5

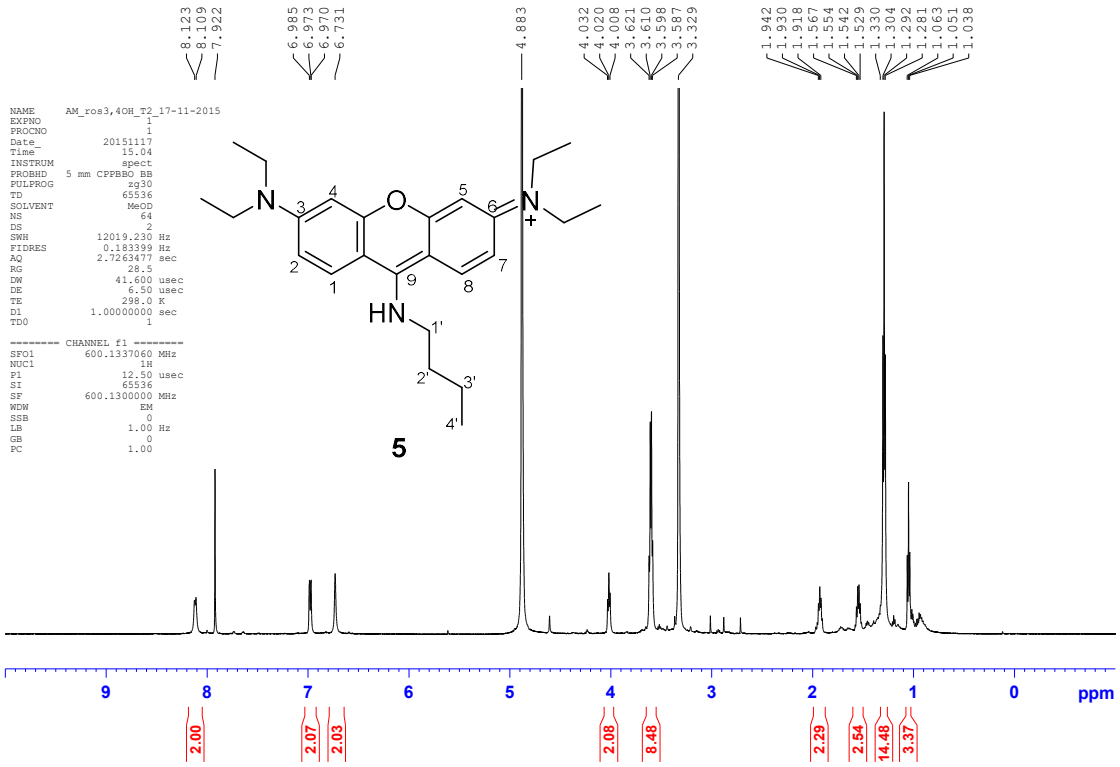


Figure S33. ^{1}H NMR spectrum (600.13 MHz, MeOD-d$_4$) of **5**.

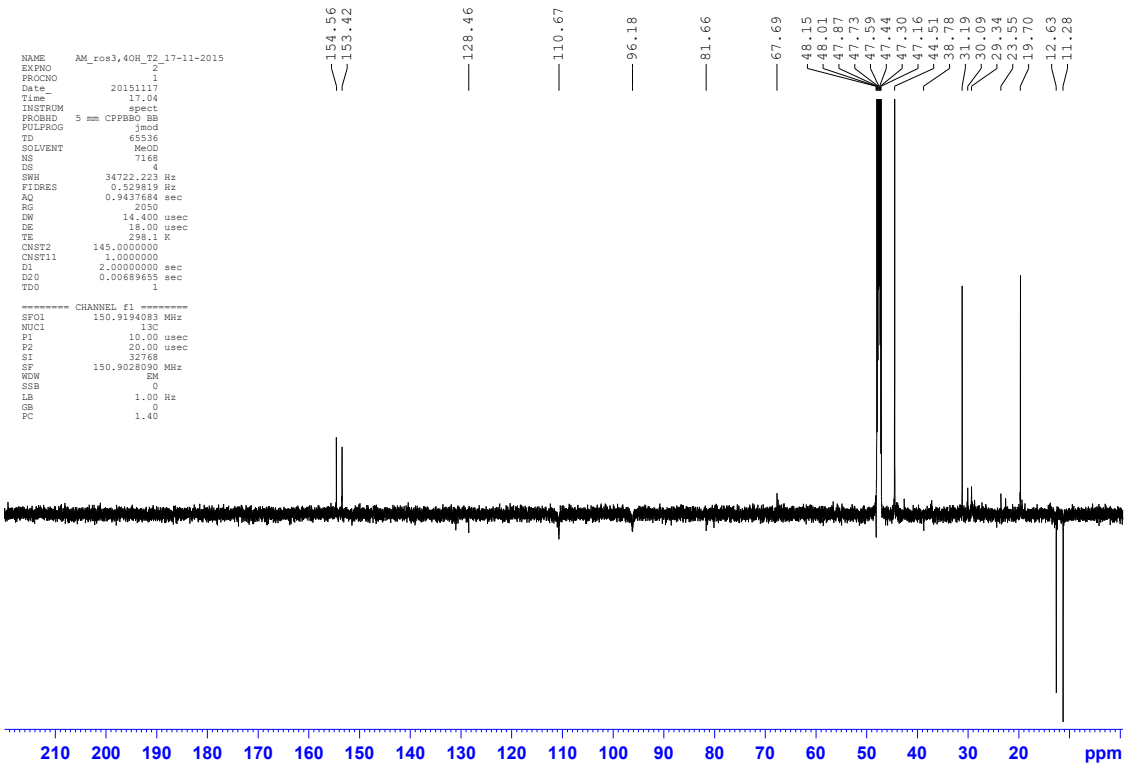


Figure S34. APT spectrum (150.90 MHz, MeOD-d$_4$) of **5**.

^{1}H NMR spectrum comparison between rosamine 4 and aminopyronin 5

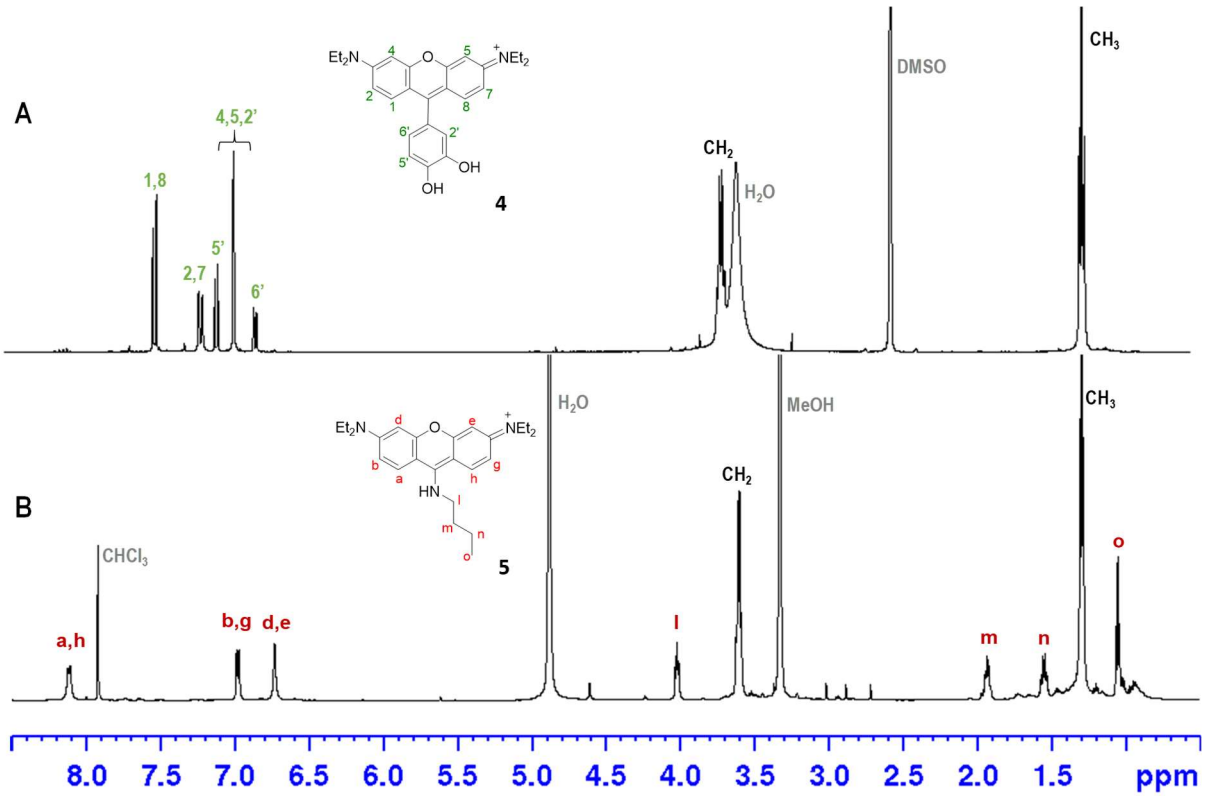


Figure S35. ^{1}H NMR spectra of **4** (A) and **5** (B).

NMR spectrum of aminopyronin 6a

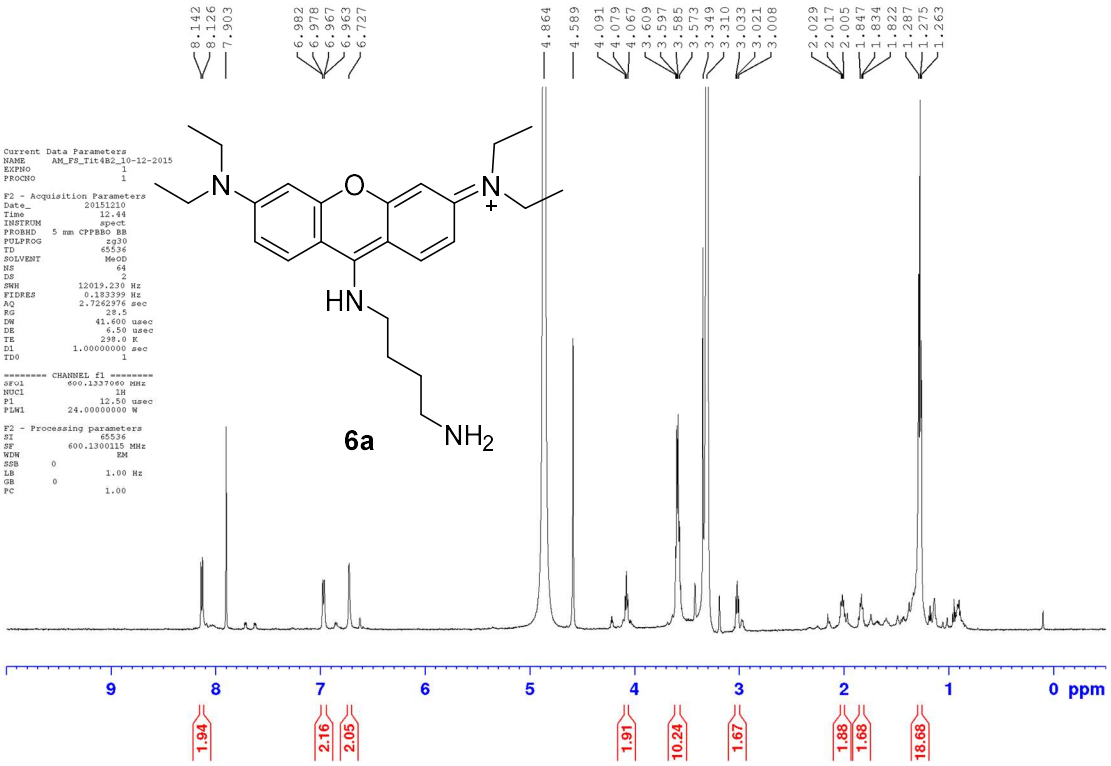


Figure S36. ^{1}H NMR spectrum (600.13 MHz, MeOD-d$_4$) of **6a**.

NMR spectrum of aminopyronin 7a

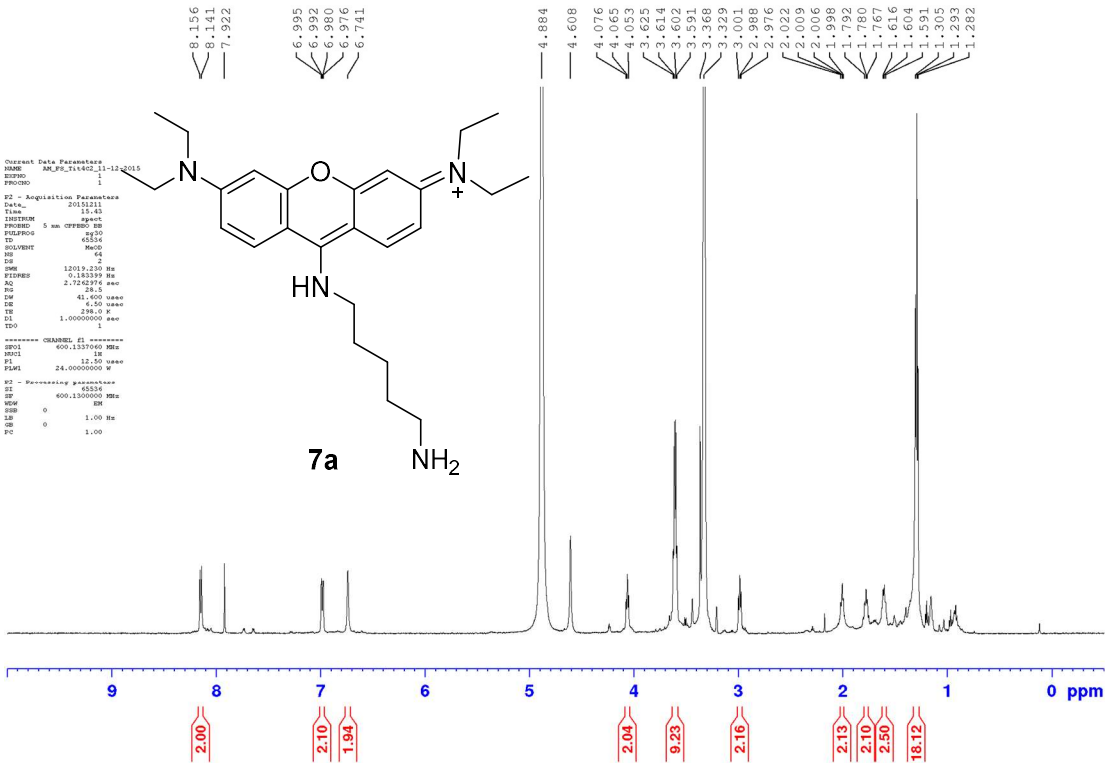


Figure S37. ^{1}H NMR spectrum (600.13 MHz, MeOD-d$_4$) of **7a**.

NMR spectrum of aminopyronin 7b

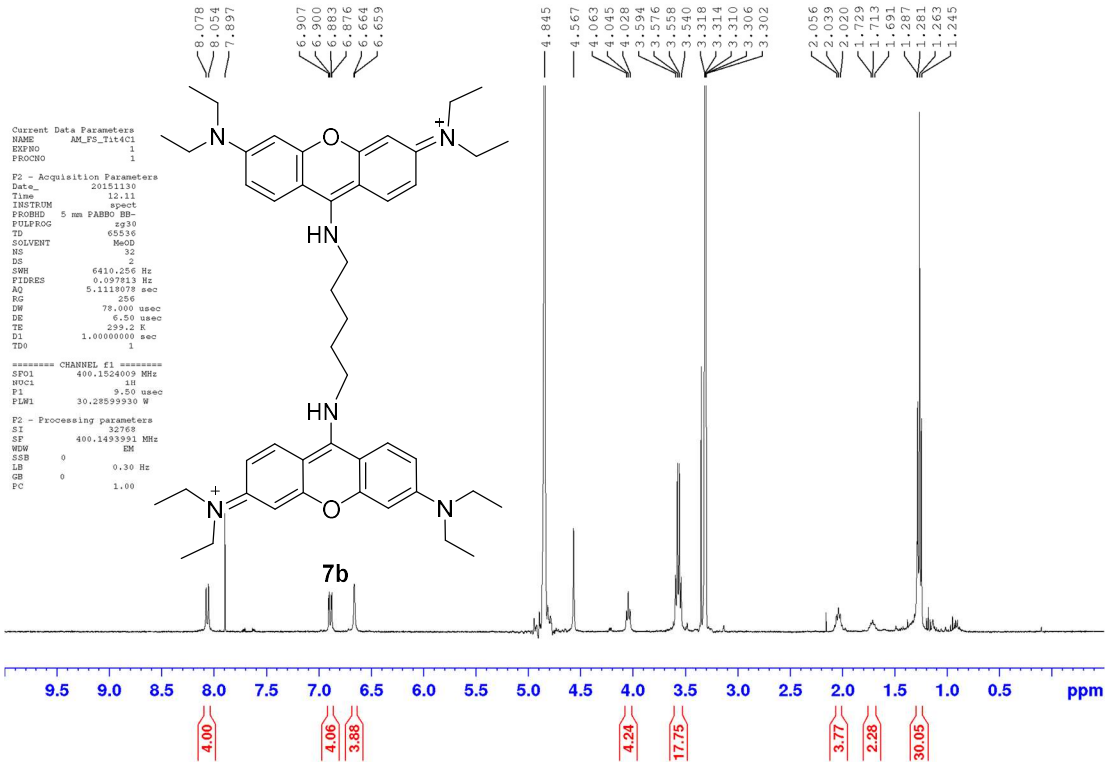


Figure S38. ^{1}H NMR spectrum (400.15 MHz, MeOD-d$_4$) of **7b**.

MS spectra of 5, 6a, 7a and 7b

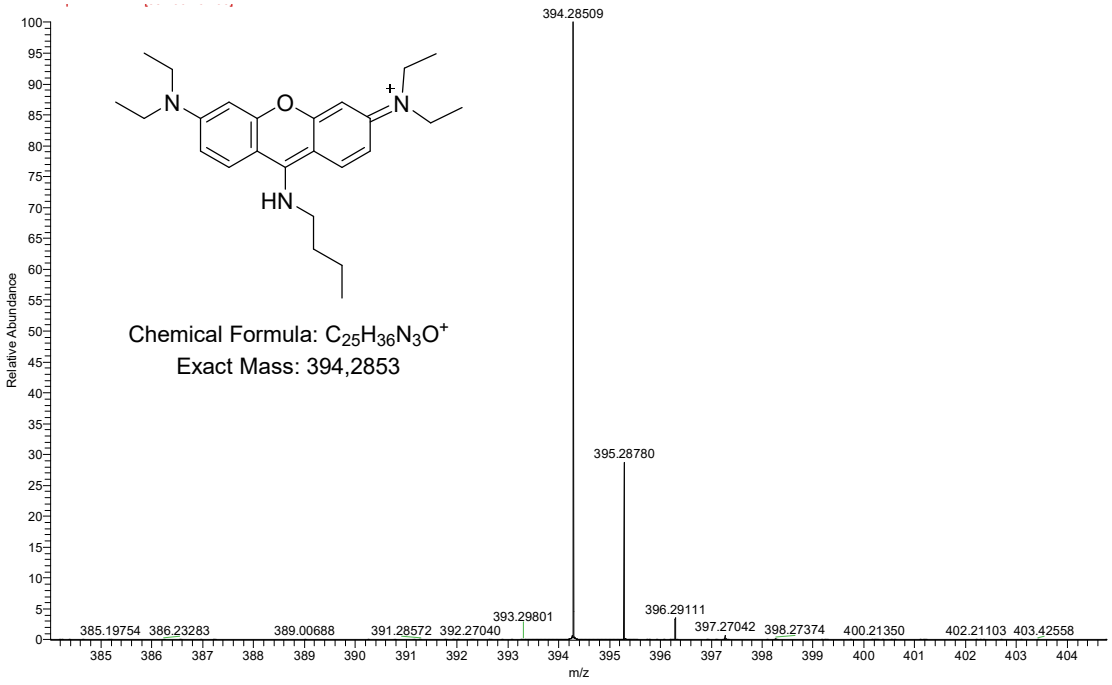


Figure S39. MS spectrum of **5**.

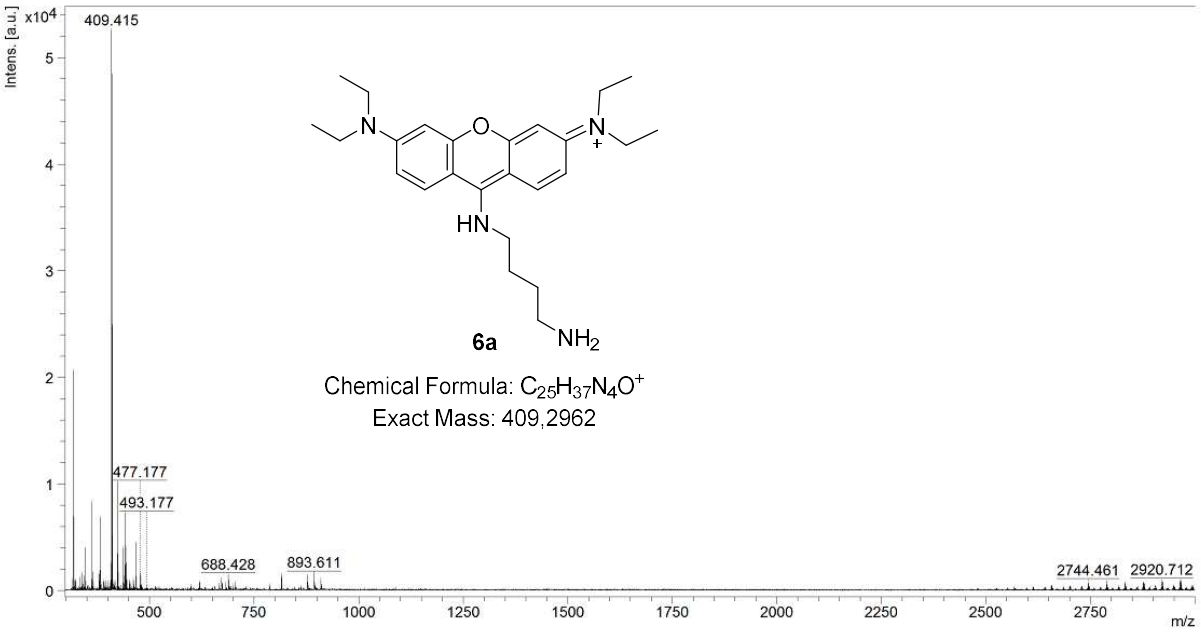


Figure S40. MS spectrum of **6a**.

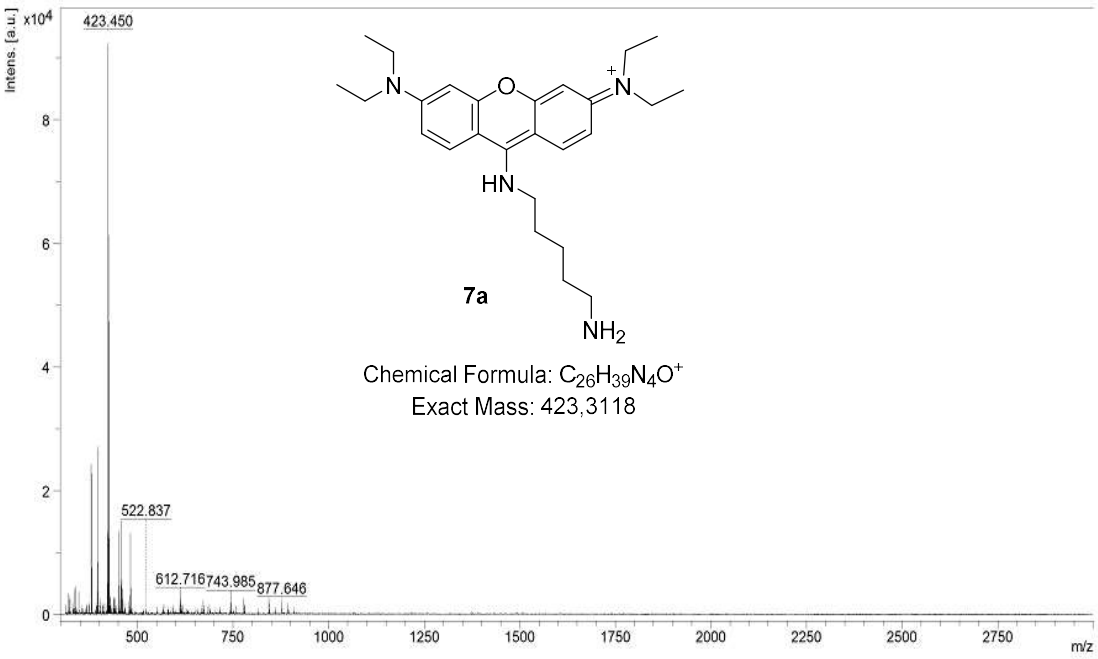


Figure S41. MS spectrum of **7a**.

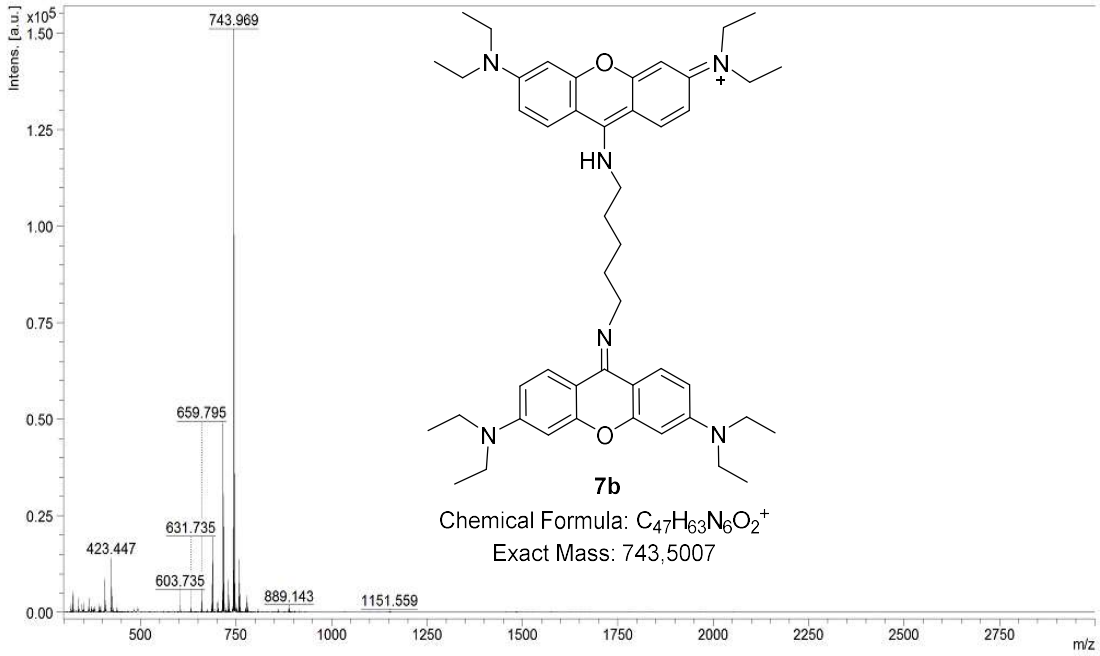


Figure S42. MS spectrum of **7b**.